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Model	Data

Weighted KNN model

5-fold CV (7	5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 353 °C

Global applicability domain: Outside

Local applicability domain index: 1.79e-01

Confidence level: 5.56e-01

Nearest Neighbors from the Training Set

Image not found

Pendimethalin Measured: 330 Predicted: 335 Image not found

Auramine
Measured: 331
Predicted: 349

Image not found

Carfentrazone-ethyl Measured: 353 Predicted: 350

Image not found

Benfluralin Measured: 370 Predicted: 349 Image not found

4,4'-Methylenebis(N,N-dimethylaniline)

Measured: 390

Predicted: 349